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**Report Title**

Multiscale Modeling and Process Optimization for Engineered Microstructural Complexity

**ABSTRACT**

This reports on the results of the MURI project on Engineering Microstructural Complexity in Ferroelectric Devices.

K. Bhattacharya, PI

## Multiscale Modeling and Process Optimization For Engineered Microstructural Complexity

### Abstract

This reports on the results of the MURI project on Engineering Microstructural Complexity in Ferroelectric Devices.

### Papers published: Peer Reviewed Journals

1. V. Gavini, J. Knap, K. Bhattacharya and M. Ortiz.  
Non-Periodic Finite-Element Formulation of Orbital-Free Density Functional Theory.  
*Journal of the Mechanics and Physics of Solids* **55**: 669-696, 2007.
2. V. Gavini, K. Bhattacharya and M. Ortiz.  
Quasi-continuum orbital-free density-functional theory: A route to multi-million atom non-periodic DFT calculation.  
*Journal of the Mechanics and Physics of Solids* **55**: 697-718, 2007.
3. K. Dayal and K. Bhattacharya.  
A real-space non-local phase-field model of ferroelectric domain patterns in complex geometries.  
*Acta Materialia* **55**: 1907-1917, 2007.
4. A. Yavari, M. Ortiz and K. Bhattacharya.  
Anharmonic lattice statics analysis of 180° and 90° ferroelectric domain walls in PbTiO<sub>3</sub>.  
*Philosophical Magazine* **87**:3997-4026, 2007.
5. A. Yavari, M. Ortiz and K. Bhattacharya.  
A theory of anharmonic lattice statics for the analysis of defective crystals.  
*Journal of Elasticity* **86**:41-83, 2007.
6. D. Shilo, E. Burcsu, G. Ravichandran and K. Bhattacharya.  
A model for large electrostrictive actuation in ferroelectric crystals.  
*International Journal of Solids and Structures* **44**: 2053-2065, 2007.
7. Y. Xiao and K. Bhattacharya.  
A continuum theory of deformable semiconducting ferroelectrics.  
*Archive for Rational Mechanics and Analysis*, In press, 2007.
8. I. Arias, S. Serebrinsky, M. Ortiz  
Cohesive model of electromechanical fatigue for ferroelectric materials and structures  
*III European Conference on Computational Mechanics (eds. C.A. Mota Soares et.al.)*, In press, 2007.
9. Q.S. Zhang, T. Cagin and W.A. Goddard, III,  
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*Proceedings of the National Academy of Sciences of the United States of America* **103**, 14695-14700, 2006.
10. Q.S. Zhang and W. A. Goddard, III,  
Charge and Polarization Distributions at the 90° Domain Wall in Barium Titanate

Ferroelectric

*Applied Physics Letters*, **89**, Art. No. 182903, 2006.

11. D. A. Boyd, L. Greengard, M. Brongersma, M.Y. El-Naggar, and D.G. Goodwin.  
Plasmon Assisted Chemical Vapor Deposition,  
*Nano Letters* **6**, 2592-2597, 2006.
12. W.-D. Yang and S. M. Haile.  
Characterization and microstructure of highly preferred oriented lead barium titanate thin films on MgO (100) by sol-gel process.  
*Thin Solid Films* **510**, 55-61 (2006).
13. M.Y. El-Naggar, K. Dayal, D.G. Goodwin and K. Bhattacharya.  
Graded ferroelectric capacitors with robust temperature characteristics.  
*Journal of Applied Physics* **100**: Art. No.114115, 2006.
14. C. Franck, G. Ravichandran and K. Bhattacharya.  
Characterization of domain walls in BaTiO<sub>3</sub> using simultaneous atomic force and piezo-response force microscopy.  
*Applied Physics Letters* **88**: Art. No.102907, 2006.
15. J.L. Ruglovsky, J. Li, K. Bhattacharya and H.A. Atwater  
The effect of biaxial texture on the effective electromechanical constants of polycrystalline barium titanate and lead titanate thin films.  
*Acta Materialia* **54**: 3657-3663, 2006.
16. I. Arias, S. Serebrinsky and, M. Ortiz  
A phenomenological cohesive model of ferroelectric fatigue,  
*Acta Materialia*, **54**: 975-984, 2006.
17. D. A. Boyd, M. Y. El-Naggar, and D. G. Goodwin.  
In Situ Measurements of Stress with Temperature in Thin Film Pb<sub>x</sub>Ba<sub>1-x</sub>TiO<sub>3</sub>  
*Journal of Integrated Ferroelectrics*, **71**: 21-28, 2006.
18. S.A. Serebrinsky, I. Arias, M. Ortiz  
Cohesive model of electromechanical fatigue for ferroelectric materials and structures  
*Mat. Res. Soc. Symp. Proc.* **902E**: Art. No. 0902-T03-07, 2006.
19. R. Zhang, D. Shilo, G. Ravichandran and K. Bhattacharya.  
Mechanical characterization of released thin films by contact loading.  
*Journal of Applied Mechanics* **7**: 730-736, 2006.
20. S. Serebrinsky and, M. Ortiz  
A hysteretic cohesive-law model of fatigue-crack nucleation  
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Depletion layers and domain walls in semiconducting ferroelectric thin films.  
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22. W.-D. Yang and S. M. Haile,  
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23. J. Li, R. Rogan, E. Üstündag and K. Bhattacharya.  
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*Nature Materials*, **4**: 776-781, 2005.
24. Y.B. Park, P. Nardi, X.D. Li and H.A. Atwater.

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*Journal of Applied Physics* **97**: Art. No. 074311, 2005.
25. R. T. Brewer, D. A. Boyd, M. Y. El-Naggar, S. W. Boland, Y.-B. Park, S. M. Haile, D. G. Goodwin, and H. A. Atwater,  
 Growth of biaxially textured Ba<sub>x</sub>Pb<sub>1-x</sub>TiO<sub>3</sub> ferroelectric thin films on amorphous Si<sub>3</sub>N<sub>4</sub>  
*Journal of Applied Physics* **97**: Art. No. 03410, 2005.
  26. W. Zhang and K. Bhattacharya.  
 A computational model of ferroelectric domains. Part I: Model formulation and domain switching.  
*Acta Materialia* **53**: 185-198, 2005.
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 A computational model of ferroelectric domains. Part II: Grain boundaries and defect pinning.  
*Acta Materialia* **53**: 199-209, 2005.
  28. M.Y. El-Naggar, D.A. Boyd, and D.G. Goodwin  
 Characterization of Highly-Oriented Ferroelectric Pb<sub>x</sub>Ba<sub>1-x</sub>TiO<sub>3</sub> Thin Films Grown by MOCVD,  
*Journal of Materials Research* **20**: 2969-2976, 2005.
  29. E. Üstündag, R.C. Rogan, M.R. Daymond, N. Tamura, L. Margulles and H. Poulson  
 Multiscale study of internal stress and texture in ferroelectrics  
*Materials Science Forum* **490-491**: 28, 2005.
  30. Y.B. Park, J.L. Ruglovsky and H.A. Atwater  
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*Applied Physics Letters* **85**: 455-457, 2004.
  31. D. Shilo, G. Ravichandran and K. Bhattacharya  
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  33. M. A. Gallivan, D. G. Goodwin, R. M. Murray  
 Effective Transition Rates for Epitaxial Growth Using Fast Modulation  
*Physical Review B*, **70**: art. no. 045409, 2004
  34. S.W. Boland, S.C. Pillai, W.D. Yang, S.M. Haile  
 Preparation of (Pb, Ba)TiO<sub>3</sub> Powders and Highly Oriented Thin Films by a Sol-Gel Process  
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 Low Temperature Crystallization of Sol-Gel Processed Pb<sub>0.5</sub>Ba<sub>0.5</sub>TiO<sub>3</sub>  
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  36. K. Bhattacharya and G. Ravichandran  
 Ferroelectric perovskites for electromechanical actuation

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37. R.T. Brewer, H.A. Atwater, J.R. Groves and P.N. Arendt  
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Texture and Strain Analysis of the Ferroelastic Behavior of Pb(Zr,Ti)O<sub>3</sub> by *In-Situ* Neutron Diffraction,  
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Rheed in-plane rocking curve analysis of biaxially-textured polycrystalline MgO films on amorphous substrates grown by ion beam-assisted deposition.  
*Applied Surface Science* **175**: 691-696, 2001
  44. M. Uludogan, T. Çagin, A. Strachan, W. A. Goddard, III  
Ab initio studies of pressure induced transitions in BaO.  
*J. Comp. Aided Material Design*, **8**,193-202, 2001.

#### **Papers published: Peer Reviewed Conference Proceedings**

1. S. W. Boland and S. M. Haile, "Oriented Ferroelectric Thin Films on Soluble Substrates," Symposium on Ferroelectricity and Piezoelectricity IMRC 2004, 22-26 Aug. 2004, Cancun, Mexico, *Integrated Ferroelectrics* **71**, 59-65 (2005).
2. S.W. Boland and S.M.Haile, "Barium Metaplumbate (BaPbO<sub>3</sub>) Electrodes for Ferroelectric Thin Films," in *Electrode Processes VII*, Editors V.I. Birss, D. Evans, M. Josowicz, and M. Osawa ECS Proceedings, Vol. 2004-18, (206<sup>th</sup> Mtg of the Electrochemical Society; Honolulu, HI, 2004; ECS, Pennington, NJ 2005) pp. 288-293.
3. S. W. Boland, and S. M. Haile, "Comparison of Titanium Precursors in the Sol-gel Synthesis of Pb<sub>0.5</sub>Ba<sub>0.5</sub>TiO<sub>3</sub> Powders and Thin Films" in *Ferroelectric Thin Films XII*, Editors D. Kaufman, S. Hoffmann-Eifert, H. Funakubo, V. Joshi, A. I.

- Kingon, I. P. Koutsaroff (Mat. Res. Soc. Symp. Proc. **784**, C11.36.1-6, Pittsburgh, PA, 2004).
4. W.-D. Yang, S. C. Pillai, S. W. Boland and S. M. Haile, "Parametric Optimization of a Sol-Gel Process for the Synthesis of Highly-Oriented (Pb,Ba)TiO<sub>3</sub> Thin Films," in *Ferroelectric Thin Films XI*, Editors D. Kaufman, S. Hoffmann-Eifert, S.R. Gilbert, S. Aggarwal, M. Shimizu (Mat. Res. Soc. Symp. Proc. **748**, U12.21.1-6, Pittsburgh, PA, 2003).

### **Papers published non-peer**

None

### **Papers Presented**

1. K. Bhattacharya gives invited presentation at the "MEMS reliability workshop" at ARL Adelphi.
2. K. Bhattacharya gives plenary lecture on "Quasicontinuum/Orbital-free density functional theory" at the International Congress of Industrial and Applied Mathematics, Zurich, 2007.
3. D.A. Boyd invited to present "Plasmon Assisted Chemical Vapor Deposition" at the International Materials Research Conference, Ferroelectrics Session, Cancun Mexico, 2007.
4. D.A. Boyd presented "Plasmon Assisted Chemical Vapor Deposition" at EuroCVD-6, Den Haag, The Netherlands, 2007.
5. D.A. Boyd presented "Plasmon Assisted Chemical Vapor Deposition" at the USC Quantum Information and Condensed Matter Physics Seminars, September 8, 2006.
6. D.A. Boyd presented "Metalorganic chemical vapor deposition of Pb<sub>x</sub>Ba<sub>1-x</sub>TiO<sub>3</sub>: Process science, diagnostics and film characterization" at the 209<sup>th</sup> meeting of the Electrochemical Society, 2006.
7. D.A. Boyd presented "Plasmon Assisted Chemical Vapor Deposition" at the 209<sup>th</sup> meeting of the Electrochemical Society, 2006.
8. D.A. Boyd presented "*In Situ* Measurements Of Stress With Temperature In Thin Film Pb<sub>x</sub>Ba<sub>1-x</sub>TiO<sub>3</sub>" International Materials Research Conference, Ferroelectrics Session, Cancun Mexico, 2005.
9. J. Ruglovsky presented "Effect of Texture Distribution on Electromechanical Behavior of Barium Titanate" in the MRS Spring Meeting, April 2005.
10. H.A. Atwater presented "Single crystal and biaxially textured perovskite thin films: Synthesis and applications" at the 2005 U.S. Army Workshop "Advanced Active Thin Film Materials For The Next Generation Of Meso - Micro Scale Army Applications" May 10-12, 2005, Florida.
11. K. Bhattacharya presented "Integrating material and machine: an attempt to develop novel ferroelectric thin film microactuators" at the 2005 U.S. Army Workshop "Advanced Active Thin Film Materials For The Next Generation Of Meso - Micro Scale Army Applications" May 10-12, 2005, Florida.

12. D.G. Goodwin presented "MOCVD growth of ferroelectric thin films" at the 2005 U.S. Army Workshop "Advanced Active Thin Film Materials For The Next Generation Of Meso - Micro Scale Army Applications" May 10-12, 2005, Florida.
13. S.M. Haile presented "Oriented LaNiO<sub>3</sub> Electrodes: Templates for Oriented Ferroelectric Thin-Films" at the 2005 U.S. Army Workshop "Advanced Active Thin Film Materials For The Next Generation Of Meso - Micro Scale Army Applications" May 10-12, 2005, Florida.
14. G. Ravichandran presented "Mechanical characterization of active thin films, at the 2005 U.S. Army Workshop "Advanced Active Thin Film Materials For The Next Generation Of Meso - Micro Scale Army Applications" May 10-12, 2005, Florida.
15. J. Ruglovsky presented "Surface Micromachining Approach to Ferroelectric MEMS Devices" at the MRS Fall Meeting 2005.
16. J. Ruglovsky presented "Theory for Effective Piezoelectric Coupling Factors for Barium Titanate and Lead Titanate Polycrystalline Films" at the MRS Fall Meeting 2005.
17. C. Franck, G. Ravichandran and K. Bhattacharya, "Characterization of domain walls using AFM & PFM on Barium Titanate" at the Society of Experimental Mechanics conference 2005 in Portland.
18. D.A. Boyd presented "*In Situ* Measurements of Macroscopic Film Stress During Growth, Cooling, and Thermal Cycling of Thin Film Pb<sub>x</sub>Ba<sub>1-x</sub>TiO<sub>3</sub>" International Materials Research Conference, Ferroelectrics Session, Cancun Mexico, 2004.
19. E. Ustundag, Internal Stresses and Constitutive Behavior of Ferroelectrics, 133rd Annual Meeting of TMS, Charlotte, North Carolina, 14-18 March 2004. Invited.
20. R. C. Rogan, "Constitutive Behavior of Pb(Zr,Ti)O<sub>3</sub> Ferroelectrics," 133rd Annual Meeting of TMS, Charlotte, North Carolina, 14-18 March 2004.
21. R. C. Rogan, "Multiscale Internal Stress Investigation of BaTiO<sub>3</sub>," 133rd Annual Meeting of TMS, Charlotte, North Carolina, 14-18 March 2004.
22. E. Ustundag, Multiscale Study of Internal Stress and Texture in Electroceramics, 106th Annual Meeting of the American Ceramic Society, Indianapolis, Indiana, 20 April 2004. Invited.
23. E. Ustundag, Multiscale Study of Internal Stress and Texture in Ferroelectrics, 7th International Conference on Residual Stress (ICRS-7), Xian, China, 14-17 June 2004. Keynote lecture.
24. E. Ustundag, "Strain and Texture Analysis of the Ferroelectric Behavior of PLZT Investigated with High Energy X-ray Diffraction," 7th International Conference on Residual Stress (ICRS-7), Xian, China, 14-17 June 2004.
25. S.A. Serebrinsky, I. Arias, M. Ortiz "Modelling of fatigue fracture in ferroelectrics", Materials Research Society - 2004 Fall Meeting, Boston, Massachusetts, December 2004.
26. Yavari, M. Ortiz, and K. Bhattacharya "Atomic structure of ferroelectric domain walls", SIAM Conference on Mathematical Aspects of Materials Science, May 23-26, 2004. Los Angeles.



27. Yavari, M. Ortiz, and K. Bhattacharya "Structure of ferroelectric domain walls in the nanoscale" 2nd International Conference on Multiscale Materials Modeling (MMM-II), October 11-15, 2004. University of California, Los Angeles.
28. Olga Kowalewsky, J. Knap, M. Ortiz, "Simulation of Cracks in Ferroelectrics using Complex Lattice Quasicontinuum" Experimental Chaos Conference (ECC8), June 14-17, 2004, Florence, Italy.
29. Olga Kowalewsky, J. Knap, M. Ortiz, "Complex Lattice Quasicontinuum Theory and Its Application to Ferroelectrics" Technical University Dresden, Germany, April 2004
30. S. Boland (invited oral) presented "Oriented Ferroelectric Thin Films on Soluble Substrates" at the International Materials Research Congress; Cancun, Mexico 2004
31. S.W. Boland, S.M. Haile, "Barium Metaplumbate ( $\text{BaPbO}_3$ ) Electrodes for Ferroelectric Thin Films" Poster at 206th Meeting of the Electrochemical Society; Honolulu, HI October 2004
32. S. W. Boland, M. Grubbs and S. M. Haile "Barium Metaplumbate ( $\text{BaPbO}_3$ ) and Lanthanum Nickelate ( $\text{LaNiO}_3$ ) Conductive Oxide Electrodes for Oriented Ferroelectric Thin Films," *Poster at MRS Fall 2004 meeting* Symposium H, Functional and Multifunctional Oxide Films.
33. D.A Boyd, Invited talk: 2004 XIII International Materials Research Congress [IMRC] August 2004.
34. K. Bhattacharya, A novel approach to microactuation in ferroelectrics, International Conference of Theoretical and Applied Mechanics ICTAM04, Warsaw, Poland, August 2004.
35. R. Rogan, Strain and Texture Analysis of the Ferroelastic Behavior of  $\text{Pb}(\text{Zr,Ti})\text{O}_3$ , 27<sup>th</sup> Annual Cocoa Beach Conference, American Ceramic Society, Cocoa Beach, FL; January 2003.
36. R. Rogan, X-Ray Microdiffraction Study of Strain Fields at Individual Domains in  $\text{BaTiO}_3$ , 27<sup>th</sup> Annual Cocoa Beach Conference, American Ceramic Society, Cocoa Beach, FL; January 2003.
37. R.C. Rogan, Microdiffraction study of the strains at domain walls in  $\text{BaTiO}_3$ , TMS annual meeting, San Diego, 3-6 March 2003.
38. R.C. Rogan, Strain and Texture analysis of  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  under compression, TMS annual meeting, San Diego, 3-6 March 2003.
39. W. Zhang and K. Bhattacharya, Modeling large strain electrostriction of ferroelectrics under combined electromechanical loads, Smart Structures and Materials 2003, San Diego 2003.
40. R. Zhang, G. Ravichandran and K. Bhattacharya, Electromechanical characterization and domain visualization during large electrostriction in ferroelectrics, Smart Structures and Materials 2003, San Diego 2003.
41. K. Bhattacharya, Materials Science Seminar, University of Southern California, 2003.
42. R.C. Rogan, Texture and Strain Analysis of PZT by In-Situ Neutron Diffraction, MRS Spring Meeting, San Francisco, CA; April 2002.
43. E. Ustundag, Constitutive Behavior of Polycrystalline Ferroelectrics, Annual Meeting of the American Ceramic Society, St. Louis, MO; May 2002.
44. R. Rogan, Ferroelastic Behavior of PZT-Based Ferroelectric Ceramics, 6<sup>th</sup> European Conference on Residual Stress, Portugal; July 2002.

45. E. Ustundag, Measurement of Strain Fields of Individual Domains in BaTiO<sub>3</sub> using X-ray Microdiffraction, 51<sup>st</sup> Denver X-ray Conference, Colorado Springs, CO; August 2002.
46. E. Ustundag, Constitutive Behavior of PZT-Based Ferroelectric Ceramics, 51<sup>st</sup> Denver X-ray Conference, Colorado Springs, CO; August 2002.
47. R. Rogan, Multiscale Characterization of Ceramics using Diffraction, (invited poster), Gordon Conference on Ceramics, August 2002.
48. D.G. Goodwin, Department Seminar, Mechanical and Aerospace Engineering, University of Southern California, 2002.
49. *Poster at MRS Fall 2002 meeting*, Symposium U, Ferroelectric Thin Films XI
50. Rhett T. Brewer, Cecily A. Ryan, Harry A. Atwater, Wein-Duo Yang and Sossina M. Haile, Biaxial Texturing and Ferroelectric Properties of Sol-gel Deposition Pb<sub>x</sub>Ba<sub>1-x</sub>TiO<sub>3</sub> on Biaxially Textured MgO *Poster at MRS Fall 2002 meeting* Symposium U, Ferroelectric Thin Films XI.
51. Wein-Duo Yang, Suresh C. Pillai, Stacey W. Boland and Sossina M. Haile, Parametric Optimization of a Sol-Gel Process for the Synthesis of Highly-Oriented (Pb,Ba)TiO<sub>3</sub> Thin Films. . *Poster at MRS Fall 2002 meeting* Symposium U, Ferroelectric Thin Films XI.
52. R. Zhang, G. Ravichandran and K. Bhattacharya, Massive Electrostriction in Barium and Lead Titanate Single Crystals, MRS Spring Meeting, San Francisco, March 4, 2002.
53. R. Zhang, G. Ravichandran and K. Bhattacharya, Observation of inner hysteresis loops of BaTiO<sub>3</sub> single crystals under electrical-mechanical loadings, USNCTAM 14 (Fourteenth U.S. National Congress of Theoretical and Applied Mechanics), June 26, 2002.
54. K. Bhattacharya, Applications of Active Materials to Microactuation , First Congress on Artificial Muscles, Albuquerque, December 02.
55. K. Bhattacharya, Domain patterns and macroscopic properties of ferroelectrics, NATO Advanced Research Workshop on New Trends in Phase Transformations and their Applications to Smart Structures, Metz, France, April 2002.
56. R. Zhang, D. Shilo, G. Ravichandran, K. Bhattacharya, Mechanical response of multilayered thin released active films, Oral presentation for SPIE, 15 March 2004.
57. R. Zhang, D. Shilo, G. Ravichandran, K. Bhattacharya, Mechanical Response of Thin Released Active Films for MEMS Actuators, SEM, 28 June 2004.
58. I. Arias, S. Serebrinsky and M. Ortiz, A cohesive model of fatigue of ferroelectric materials under electro-mechanical cyclic loading, SPIE 11th Annual International Symposium on Smart Structures and Materials, San Diego, 2004.
59. I. Arias, S. Serebrinsky and M. Ortiz, Fatigue behavior of ferroelectrics, SIAM Conference on Mathematical Aspects of Materials Science, Los Angeles, 2004.
60. MRS Fall Meeting (poster presentation):  
S.W. Boland and S.M. Haile, Comparison of Titanium Precursors in the Sol-Gel Synthesis of Pb<sub>0.5</sub>Ba<sub>0.5</sub>TiO<sub>3</sub> Powders and Thin Films poster presentation at Fall 2002 MRS meeting, in *Ferroelectric Thin Films XII*, Boston, 1-4 December 2003.
61. S.M. Haile, S.W. Boland and W.-D. Yang, "Sol-gel Synthesis of Oriented Ferroelectric Thin Films" oral presentation at ARL/ARO-Caltech MURI Workshop, Adelphi, 4 December 2003.

62. S.W. Boland, W.-D. Yang and S.M. Haile, "Sol-Gel Synthesis of Highly-Oriented Ba<sub>0.5</sub>Pb<sub>0.5</sub>TiO<sub>3</sub> Thin Films" poster presentation at ARL/ARO-Caltech MURI Workshop, Adelphi, 4 December 2003.
63. S.W. Boland and S.M. Haile, "Sol-Gel Synthesis of Highly-Oriented Ba<sub>0.5</sub>Pb<sub>0.5</sub>TiO<sub>3</sub> Thin Films," poster presentation at WEST sponsored meeting "2003 Graduate Science Symposium," Pasadena, 11 November 2003.
64. R.T. Brewer, D.A. Boyd, M. El-Naggar, S.W. Boland, S.M. Haile, D.G. Goodwin and H.A. Atwater, Ion-Beam Assisted Deposition of Biaxially Textured MgO on Amorphous Si<sub>3</sub>N<sub>4</sub> for Heteroepitaxy of Biaxially Textured BaXPb<sub>1-x</sub>TiO<sub>3</sub> 204th Meeting of the Electrochemical Society; Orlando, FL October 2003.
65. S.W. Boland and S.M. Haile, Comparison of Titanium Precursors in the Sol-Gel Synthesis of Pb<sub>0.5</sub>Ba<sub>0.5</sub>TiO<sub>3</sub> Powders and Thin Films poster presentation at Fall 2002 MRS meeting, in *Ferroelectric Thin Films XII*, Boston, 1-4 December 2003.
66. S.M. Haile, S.W. Boland and W.-D. Yang, "Sol-gel Synthesis of Oriented Ferroelectric Thin Films" oral presentation at ARL/ARO-Caltech MURI Workshop, Adelphi, 4 December 2003.
67. S.W. Boland, W.-D. Yang and S.M. Haile, "Sol-Gel Synthesis of Highly-Oriented Ba<sub>0.5</sub>Pb<sub>0.5</sub>TiO<sub>3</sub> Thin Films" poster presentation at ARL/ARO-Caltech MURI Workshop, Adelphi, 4 December 2003.
68. S.W. Boland and S.M. Haile, "Sol-Gel Synthesis of Highly-Oriented Ba<sub>0.5</sub>Pb<sub>0.5</sub>TiO<sub>3</sub> Thin Films," poster presentation at WEST sponsored meeting "2003 Graduate Science Symposium," Pasadena, 11 November 2003.
69. R.T. Brewer, D.A. Boyd, M. El-Naggar, S.W. Boland, S.M. Haile, D.G. Goodwin and H.A. Atwater, Ion-Beam Assisted Deposition of Biaxially Textured MgO on Amorphous Si<sub>3</sub>N<sub>4</sub> for Heteroepitaxy of Biaxially Textured BaXPb<sub>1-x</sub>TiO<sub>3</sub> 204th Meeting of the Electrochemical Society; Orlando, FL October 2003.
70. D.A. Boyd, MRS Fall 2003: poster.
71. D.A. Boyd, ARL Workshop: Fall 2003.
72. D.A. Boyd, APS Spring 2003; talk.
73. D.A. Boyd, ECS Spring 2003; talk.
74. E. Ustundag, "Measurement of strain fields around domains in BaTiO<sub>3</sub> using x-ray microdiffraction," 52nd Denver X-ray Conf, Denver CO; 4-8 August 2003.
75. E. Ustundag, "Constitutive Behavior of Electroceramics," IMI Workshop, Knoxville, TN, Nov. 2003. Invited.
76. E. Ustundag, Micromechanics of Domains in BaTiO<sub>3</sub> Studied by Polychromatic Scanning X-ray Microdiffraction, Frontiers of X-Ray Micro and NanoBeam Diffraction Symposium, TMS MS&T '03: Materials Science & Technology, Chicago, Illinois, 9-12 November 2003. Invited.
77. W.D. Yang, S.C. Pillai, S.W. Boland, S. M. Haile, Parametric Optimization of a Sol-Gel Process for the Synthesis of Highly-Oriented (Pb, Ba)TiO<sub>3</sub> Thin Films poster presentation at Fall 2002 MRS meeting, in *Ferroelectric Thin Films XI*, Boston, 2-5 December 2002.
78. W.D. Yang, S.C. Pillai, S.W. Boland, S. M. Haile, Parametric Optimization of a Sol-Gel Process for the Synthesis of Highly-Oriented (Pb, Ba)TiO<sub>3</sub> Thin Films poster

presentation at Fall 2002 MRS meeting, in *Ferroelectric Thin Films XI*, Boston, 2-5 December 2002.

## **Books**

None

## **Honors**

1. M. Ortiz is elected Fellow of the American Academy of Arts and Sciences, 2007.
2. G. Ravichandran awarded Doctor Honoris Causa (Dhc) by the Paul Verlaine University, 2006
3. G. Ravichandran has been named Goode Professor of Aeronautics and Mechanical Engineering, 2006.
4. K. Bhattacharya has been named Midwest Mechanics Lecturer, 2006-2007.
5. M. Ortiz delivers the Penner Distinguished Lecture, UC San Diego, 2006.
6. M. El-Naggar has received a Applied Materials fellowship, 2006.
7. R. Zhang received the Coles Award for most innovative experimental design by a doctoral candidate, 2005.
8. G. Ravichandran has been awarded the Lazan Award of the Society of Experimental Mechanics.
9. E. Burscu, G. Ravichandran and K. Bhattacharya received the Best paper in Active Materials award from ASME, 2004.
10. M. Ortiz has been granted the Humboldt Research Award for Senior U.S. Scientists, 2002.
11. Stacey Boland received the Intel Graduate Student Fellowship, 2004-05
12. Stacey Boland received a PEO Scholar Award, 2005
13. Melody Grubbs received a Melon Minority Fellowship, 2005
14. Jennifer Ruglovsky received the Applied Materials Fellowship, 2004-05
15. Mohammed El-Naggar received the Applied Materials Fellowship, 2004-05
16. S.M. Haile presented the MSE DOW Lecture at Northwestern University, 2005
17. G. Ravichandran appointed as the John E. Goode, Jr. Professor of Aeronautics and Mechanical Engineering, 2005
18. G. Ravichandran awarded the Lazan Award of the Society of Experimental Mechanics, 2005.
19. E. Ustundag: Keynote speaker, 7th International Conference on Residual Stress (ICRS-7), Xian, China, 2004.
20. E. Ustundag: Elected member of the Advanced Photon Source Scientific Program Advisory Committee, 2004.
21. K. Bhattacharya awarded the Young investigator award by the Society of Engineering Sciences, 2004.
22. K. Bhattacharya awarded the Special Achievements Award in Applied Mechanics by the American Society of Mechanical Engineers, 2004.
23. K. Bhattacharya, G. Ravichandran and E. Burscu awarded the Best Paper award by the Smart Structures Division of the American Society of Mechanical Engineers, 2004.
24. R. C. Rogan: NSF International Materials Institute Fellowship, 2003.

25. R. C. Rogan: Best Student Presentation, Meca-Sens 2003, 2<sup>nd</sup> International Conference on Stress Evaluation by Neutron and Synchrotron Radiation, 2003.
26. R.M. Murray is the plenary speaker at the European Controls Conference, September 2003.
27. M. Ortiz is the plenary speaker at International Conference on Industrial and Applied Mathematics (ICIAM-2003) in Sydney, 2003.
28. H.A. Atwater is the plenary speaker at the Electronic Materials Symposium 2002
29. M. Ortiz was the plenary speaker at the World Congress on Computational Mechanics in Vienna, 2002.
30. W.A. Goddard, III invited speaker at the Workshop on Fundamental Physics of Ferroelectrics, 2002.
31. K. Bhattacharya and his research profiled in Business Week (Jan 4, 2002) ([http://www.businessweek.com/technology/content/jan2002/tc2002014\\_7459.htm](http://www.businessweek.com/technology/content/jan2002/tc2002014_7459.htm))
32. W.A. Goddard, III awarded the Tolman Prize from the Southern California Section of the American Chemical Society, 2001.
33. G. Ravichandran received one year visiting fellowship at Ecole Polytechnique as Directeur de Recherche, CNRS, France, 2001.
34. H.A. Atwater appointed as Howard Hughes Professor of Applied Physics, 2001.
35. R.T. Brewer awarded the Intel fellowship, 2001.
36. W.A. Goddard, III named as one of the 99 most Highly Cited Chemists from 1981 to 1999 (<http://isihighlycited.com>)

## Patents

1. H.A. Atwater, K. Bhattacharya, K. Dayal, M. Dicken, D. Psaltis, G. Ravichandran and A. Scherer.  
Ferroelectric nanphotonic materials and devices.  
US and PCT Patent Application, Filed 2006.
2. L.F. Greengard, M. Brongersma, D.A. Boyd.  
Method and system for forming a film of material using plasmon assisted chemical reactions.  
US Patent Application, Filed 2005.
3. L.F. Greengard, M. Brongersma, D.A. Boyd.  
Electromagnetic control of chemical catalysis.  
US Patent Application, Filed 2005.
4. R Zhang, D. Shilo, G. Ravichandran and K. Bhattacharya.  
Method and apparatus for measuring the mechanical response of micro-electro-mechanical systems. Filed, 2005.

## Scientific Progress

*Quasi-continuum orbital-free density-functional theory: A route to multi-million atom non-periodic DFT calculation*

- Density functional theory has provided insights into various materials properties in the recent decade. However, the computational complexity of this approach has made other aspect, especially those involving defects, beyond reach. We have developed a

method that enables the study of a multi-million atom cluster using orbital free density functional theory with no spurious physics or restrictions on geometry. The key idea is a systematic means of adaptive coarse-graining retaining full resolution where it is necessary and coarsening with no patches, assumptions or structure. We demonstrate the method, its accuracy under modest computational cost and the physical insights it offers using a multi-million cluster of aluminum containing a single defect.

#### *Synthesis of textured electrode and ferroelectric films using sol-gel*

- Synthesized out-of-plane oriented  $\text{LaNiO}_3$  conducting oxide electrodes on a variety of substrates [ $\text{Si}(111)$ ,  $\text{Si}(100)$ ,  $\text{Si}_3\text{N}_4$ ,  $\text{Ti/Si}$ ,  $\text{Pt/Ti/SiO}_2/\text{Si}$ ,  $\text{SiO}_2/\text{Si}$ , and  $\text{SiO}_2$ ] by chemical solution deposition (CSD) methods. Sheet resistance shown to be sufficient for electrode applications,  $\sim 50 \Omega/\text{square}$  under ambient conditions. Demonstrated that texturing occurs by a classic mechanism in which grains exposing low energy, slow-growing surfaces eventually dominate the film. Absence of in-plane orientation revealed by X-ray diffraction pole figure analysis.
- Deposited oriented  $\text{Ba}_x\text{Pb}_{1-x}\text{TiO}_3$  and PZT on oriented  $\text{LaNiO}_3$  conducting oxide electrodes by CSD. Demonstrated robustness of  $\text{LaNiO}_3$  as a CSD substrate as compared to  $\text{MgO}$  for the deposition of  $\text{Ba}_x\text{Pb}_{1-x}\text{TiO}_3$  as a result of the lower sensitivity of  $\text{LaNiO}_3$  to atmospheric moisture.  $\text{Ba}_x\text{Pb}_{1-x}\text{TiO}_3$  crystallization temperature reduced to  $450^\circ\text{C}$ .
- Carried out extensive surveys of alternate chemical systems (alternate precursors and solvents) to enhance in-plane orientation of  $\text{LaNiO}_3$  attainable by CSD. Some promising systems have emerged, but as yet none provide sufficient bi-axial orientation. Exploration of CSD parameter space continues.

#### *Synthesis of textured electrode and ferroelectric films using pulsed laser deposition*

- Synthesized biaxially textured films  $\text{Ba}_x\text{Pb}_{1-x}\text{TiO}_3$  with  $\text{SrRuO}_3$  electrodes. As grown films are oxygen-deficient with poor properties, and thus are oxygenated by annealing in an oxygen rich atmosphere. The films have been demonstrated to have biaxial texture, excellent ferroelectric and switching behavior under piezo-force microscopy (PFM) and good optical quality.

#### *Fabrication and testing of ferroelectric bridges and cantilevers*

- Fabricated a series of bridge like test-structures with various controls:
  - $\text{PT/Au/SiO}_2$  using MOCVD
  - $\text{PT/Au/SiO}_2$  using PLD (unfortunately gave wrong phase)
  - $\text{PT/MgO/SiO}_2$  using MOCVD (good quality but no bottom electrode)
  - $\text{PT/SRO/MgO/SiO}_2$  using PLD
- The bridges are tested using a variety of means
  - Force-displacement-voltage testing using the electromechanical test-bed. The mechanical tests are extremely repeatable, and allow us to extract residual stress and elastic modulus.
  - Cracking behavior using the electromechanical test-bed.
  - Cathodoluminescence measurements on films to explore microstructure (new application of this technique)

- PFM
- The role of texture in enhancing piezoelectric response demonstrated

#### *Plasmon Assisted Chemical Vapor Deposition*

- We introduce a new chemical vapor deposition (CVD) process that can be used to selectively deposit materials of many different types. The technique makes use of the plasmon resonance in nanoscale metal structures to produce the local heating necessary to initiate deposition when illuminated by a focused low-power laser. We demonstrate the technique, which we refer to as plasmon-assisted CVD (PACVD), by patterning the spatial deposition of PbO and TiO<sub>2</sub> on glass substrates coated with a dispersion of 23 nm gold particles. The morphology of both oxide deposits is consistent with local laser-induced heating of the gold particles by more than 150 °C. We show that temperature rises of this magnitude are consistent, considering the heat loss mechanisms. The technique is general and can be used to spatially control the deposition of virtually any material for which a CVD process exists.

#### *Fundamental studies of ferroelectric materials*

- Study the Variation of Phonon distortion to understand diffuse scattering, and found that it is related to a TO-TA transformation during the symmetry reduction from Pm3m to I-43m. The TA modes in I-43m are anisotropic and always softer than TO modes, leading to observed diffuse X-ray scattering.
- Developed the PQEq force field based on QM calculations for BaTiO<sub>3</sub>, which enabled us to extend first principles based calculations to over 5000 atoms. This allowed us to determine the equilibrium structure of the 90° domain walls for periodic cells with lengths up to 74 nm (5120 atoms). We find that the domain wall has a width of 21 nm consisting of a dramatic switch in polarization over a 5 nm central layer surrounded by two transition layers each 8 nm wide. The central 5nm layer consists of a 2 nm sublayer with overshooting polarizations and a 3 nm sublayer with reversed polarization. This structure explains the discrepancies in interpreting previous experimental and theoretical analyses of the domain width and provides a great deal of detailed information about distortions, charges, and electric field that we be of great interest to workers in the field. In particular we find that long-range interactions are crucial in stabilizing the domain wall.
- Anharmonic lattice statics calculations show that a periodic array of oxygen vacancies on a 180-degrees domain wall make its thickness double. This is the first quantitative calculation that shows domain wall broadening due to oxygen vacancies. This is in agreement with recent experimental studies by Shilo et al. (2004).

#### *Theoretical models of electromechanical fatigue*

- Developed a cohesive model for electromechanical fatigue and provided a thorough comparison with experimental data. The local hysteretic cohesive model was embedded into a simple slab geometry, and we considered the variation of a number of system parameters, to wit, number of applied cycles, nominal field amplitude, slab thickness and applied field frequency. In particular, we concluded that the exhaustion of the effective applied field due to the degrading cohesive interfaces, which is responsible for the size effect, also leads to a decrease in the amount of switching

with increasing field frequency. This is in line with several reported experimental data.

#### *Modeling of Compositionally-Graded Ferroelectrics.*

- In preparation for experimental studies on the growth and dielectric properties of graded  $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$  thin films, we developed a continuum model that accounts for the spatial variation in properties and the long-range electrostatic interactions in functionally graded ferroelectrics, with an emphasis on the dielectric behavior. Two geometries are emphasized as case studies; parallel electrode and interdigitated electrode configurations. In both cases, we look for solutions of the polarization nominally aligned with the applied electric field, and compute the temperature-dependent dielectric response. We find that the parallel electrodes configuration results in a strong temperature-dependence of the dielectric constant, due to the strong electrostatic interactions between the different layers. On the other hand, interdigitated electrodes lead to a parallel capacitance geometry that results in a broad phase transition with temperature, as is desired for tunable filter applications.

#### *Phase-field modeling of ferroelectric devices.*

- Developed a phase field approach that can study domain patterns and domain evolution in complex geometries with no *a priori* assumption on geometry, electrode arrangement and dielectric properties. While modern devices utilize domain switching in complex geometries and electrode arrangements, current models of domain evolution make assumptions like periodicity and complete shielding. Our work overcomes these restrictions. The key idea is a boundary element method to resolve the electrostatic fields. We use the method to examining the closure domains that form at a free surface, domain switching under cyclic electric field in a device with interdigitated electrodes and domain switching at a notch.

#### **Contacts with DoD personnel.**

1. Melanie Cole from ARL has spent a sabbatical at Caltech collaborating with David Goodwin, David Boyd, Kaushik Bhattacharya and others in the MURI group. She is developing a MOCVD system modeled after the system developed in the Goodwin lab at Caltech. Further, the theoretical work on graded BST films is the basis of an experimental effort on her part to synthesize graded BST films via MOCVD in collaboration with Goodwin and Boyd. In addition, Melanie Cole has explored the possibility of incorporating oriented  $\text{LaNiO}_3$  electrodes developed by Stacey Boland and Melody Grubbs (Haile group) in BST based thin-film devices.
2. K. Bhattacharya gives invited presentation at the “MEMS reliability workshop” at ARL Adelphi.
3. H.A. Atwater, K. Bhattacharya, D.G. Goodwin, S.M. Haile and G. Ravichandran presented invited talks at the 2005 U.S. Army Workshop “Advanced Active Thin Film Materials For The Next Generation Of Meso - Micro Scale Army Applications” May 10-12, 2005, Florida.
4. Dr. Melanie Cole visited Caltech on July 15, 2004, presented a very well-attended seminar and held discussions with various MURI team members.



5. Joint ARL-Caltech workshop in Army Research Lab, Adelphi MD organized by Drs. Madan Dubey, ARL and G. Ravichandran, Caltech. Speakers included John Prater and William Lampert, ARO; Harry Atwater, Sossina Haile, David Goodwin, Ersan Ustundag, Guruswami Ravichandran, Tahir Cagin, Kaushik Bhattacharya, Caltech; Peter Chung, Frank Crowne, Melanie Cole, John Demaree, Eric Ngo, ARL; David Singh, NRL; and attendees included G. Ravichandran, Caltech; Jeff Pulskamp, Luke Currano, ARL; David A. Boyd, Santiago A. Serebrinsky, Jennifer Ruglovsky, Robert Rogan, Caltech; Eric Ngo, Eugene Zakar, Madan Dubey, Alma Wickenden, Frank Crowne, ARL; Stacey W. Boland, Caltech; Derek Demaree, Daniel Potrepka, Gary Hirsch, Peter W. Chung, Raju Namburu, Steven Tidrow, Roland Polcawich, ARL; Tahir Cagin, Sossina Haile, David Goodwin, Kaushik Bhattacharya, Harry Atwater, Caltech; Bill Lampert, John Prater, ARO; Qingsong Zhang, Caltech; Melanie Cole, ARL; David Singh, NRL. The workshop included both talks as well as informal discussion brain-storming session. Three concrete areas of collaboration emerged and are progressing. December 4, 2003.
6. Jennifer Ruglovsky using ARL, Adelphi facilities (Point of contact: Dr. Brett Piekarski, ARL) for microactuator synthesis, 2003-04.
7. David A. Boyd interacts with Dr. Alma Wickenden (ARL) for development and fabrication of PBT microstructures, 2003-04.
8. Review meeting in Caltech. B. Lampert (ARO), J. Prater (ARO) and M.W. Cole (ARL) visited Caltech on October 10, 2003.
9. Kickoff-meeting. M. Dubey (ARL), J. Prater (ARO), M. Zikry (ARO), D. Singh (NRL), J. Wu (ARO), A. Amin (NUWC), M.W. Cole (ARL), W. Mullins (ARO), S. Tidrow (ARL) visited Caltech on Wednesday May 30, 2001.
10. Review Meeting. B. Lampert (ARO), J. Prater (ARO), M.W. Cole (ARL), W. Mullins (ARO), visited Caltech on October 9, 2002.
11. S. Boland, graduate student, visited Army Research Lab, Adelphi MD September 10-14, 2001 for a week-long working visit with A. Wickenden.
12. A. Wickenden (ARL) visited Caltech during the week of July 8, 2002 for collaborative research projects with the PIs and co-PIs.
13. K. Bhattacharya, PI visited the Army Research Lab, Adelphi MD, Dec. 10, 2001. Gave a research presentation and participated with a round-table meeting with M. Dubey (ARL), J. Prater (ARO), C. Chabalowski (ARL), E. Zakar (ARL), H.A. Hung (ARL), D. Novotny (ARL), T. Takaci (ARL), D. Smith (ARL), G. McLane (ARL), B. Piekarski (ARL), S. Karamchetty (ARL), J. Pulsanp (ARL), J. Little (ARL), M.H. Ervin (ARL), A. Wickenden (ARL), P. Cheung (ARL).
14. K. Bhattacharya, PI visited the Naval Research Lab, Washington DC, Dec. 11, 2001. Gave research presentation and held meetings with D. Singh (NRL).
15. R.M. Murray has joined the Air Force Scientific Advisory Board.

#### **Faculty and Senior Researchers**

H.A. Atwater, K. Bhattacharya, W.A. Goddard III, D.G. Goodwin, S.M. Haile, M. Ortiz, G. Ravichandran, E. Üstündag, R.M. Murray, T. Cagin, J. Knap

#### **Grad Students**

K. Dayal, J. Ruglovsky, M. Dicken, K. Diest, Q.S. Zhang, M. El-Naggar, S. Boland, G. Sukul, A. Kelly, O. Schneider, A. Yavari, V. Gavini, R. Zhang, R. Hockersmith, V. Deshpande, R. T. Brewer, C. Ryan, B. Kaufman, M. Ulundogan, M.A. Gallivan, R. Brockwell, G. Rosene, R.C. Rogan, S.M. Motahari, V. Gavini

**Post Doctorates**

Y. Xiao, Y-B. Park, Q.S. Zhang, D.A. Boyd, S. Serebrinsky, I. Arias, R. Zhang, R. Kunnath, W. Zhang, A. Strachan, S. Pillai, W-D Yang,

**Master Degrees**

S. Boland, M. Dicken, K. Diest, M. El-Naggar, S. Boland, G. Sukul, O. Schneider, A. Yavari, V. Gavini, R. Zhang

**Under Graduates**

M. Grubbs, J. Messenger, R. Abraham, A. Subramaniam, S. Gao, K. Hammond

**Doctorate Degrees**

Y. Xiao, K. Dayal, R.T. Brewer, Q.S. Zhang, S. Boland, M.A. Gallivan, O. Schneider, A. Yavari, R.C. Rogan, R. Zhang, J. Ruglovsky, M. El-Naggar, S.M. Motahari, V. Gavini.